

The Long-Wavelength Limit of the Bhatia – Thornton Structure Factor “Concentration – Concentration” in Liquid Na-K

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Abstract

The concentration dependency of the Bhatia-Thornton structure factor “concentration - concentration” in the long-wavelength limit for the liquid system Na-K is calculated by using the variational method in conjunction with the pseudopotential one. Our results confirm smoothness of the dependency under consideration obtained experimentally by Caffasso *et al.* (1967) and by Alblas *et al.* (1980), although numerically our results lie closely to experiment of Hultgren *et al.* (1973).

Keywords: Bhatia-Thornton structure factors, Na-K liquid alloy, pseudopotential theory, variational method

In a binary mixture the Bhatia-Thornton [1] structure factor “concentration - concentration”, $S_{cc}(q)$, can be expressed in terms of the Ashcroft-Langreth [2] partial structure factors, $S_{ij}(q)$, as follows:

$$S_{cc}(q) = c_1 c_2 [c_2 S_{11}(q) + c_1 S_{22}(q) - 2\sqrt{c_1 c_2} S_{12}(q)] \quad , \quad (1)$$

where c_i is the concentration of the i -th component.

The concentration dependency of this characteristic in the long-wavelength limit shows has or no a system under consideration the tendency to the phase separation or to strong association.

Here, we investigate $S_{cc}(0)$ for liquid system Na-K at $T=373\text{K}$ in the framework of the standard variational method [3] of the thermodynamic perturbation theory. For this aim, the local Animalu-Heine [4] model pseudopotential and the Vashishta – Singwi [5] exchange–correlation function are used. Earlier, this method was successfully used for thermodynamics study of liquid binary alloys of alkali metals [6].

Obtained results in comparison with experimental data are represented in Fig.1. The agreement with experiments is quite satisfactory. Absolute values calculated at different concentrations better agree with experimental results of work [7], whereas the calculated curve behavior better agree with results [8, 9].

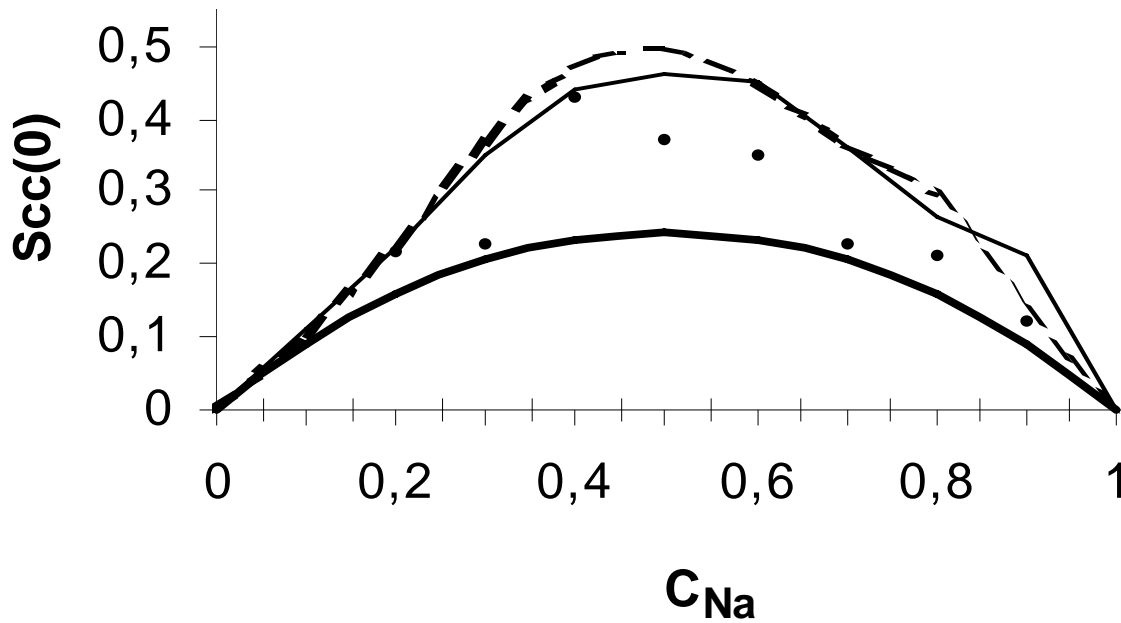


Figure 1. $S_{cc}(0)$ of liquid Na-K at $T=373\text{K}$ (bold full line – our result; full line – experiment [7]; dotted line – experiment [8]; circles – experiment [9]).

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